

## Dispersion spectra of FCC metals (Pt, Pb and Th)

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A new five parameter model for the lattice dynamical behaviour of cubic metals (FCC) have been developed. The ion-ion interactions, being purely central, have been described in terms of radial and transversal force components associated with first and second neighbouring ions. An equilibrium condition has been derived in terms of the transversal components. The ion-electron-ion interactions have been included on the basis of Sharma-Joshi scheme, which can be handled easily computationally. The dispersion frequencies for platinum, lead and thorium (FCC) have been computed on the basis of the model.

### 1. INTRODUCTION

In the recent past DeLaunay (1956), Clark *et al* (1964), Yuen & Varshni (1967), Varshni & Yuen (1968) and Konti (1971) have examined the feasibility of assuming the angular forces in order to account the Cauchy's discrepancy. Behari & Tripathi (1969, 1970, 1971, 1972) have combined the ion-electron-ion interactions with the angular interactions to explain the lattice dynamical behaviour of the metals.

The dispersion spectra of the metals (platinum, lead and thorium) considered here require more successful explanation of their crystal-dynamics. It is also worth-realising that angular forces were thought of as forces arising from inter-bond interactions between covalent bonds and hence there is hardly any justification in talking about angular forces in case of metals.

In view of this we have developed a five parameter model containing radial and transversal central interaction terms for nearest and next nearest neighbouring ions. An equilibrium condition has been derived considering total pressure due to ions and electrons. The ion-electron-ion interactions have been included on the basis of simple Sharma-Joshi (1963) scheme.

### 2. THEORY

The central pair potential (CPP) model developed here expresses the total potential energy ( $\phi$ ) of the crystal as the sum of Coulombian ion-ion energy ( $\phi^i$ ) and ion-electron ion energy ( $\phi^e$ ) i.e.,

$$\phi = \phi^i + \phi^e. \quad \dots \quad (1)$$

The ion-ion energy ( $\phi$ ) is the sum of total potential due to nearest and next-nearest neighbouring ions. Thus,

$$\phi = \frac{1}{2} \sum_j \phi^i(R_j) + \phi^e. \quad \dots (2)$$

The crystal exist in static equilibrium under zero external stress. Considering the ions as the points located in the sea of electrons, the first derivative of total energy ( $\phi$ ) with respect to atomic volume ( $V$ ) should vanish, i.e.,

$$\left| \frac{\partial \phi}{\partial V} \right| = 0 \quad \dots (3)$$

on evaluation we get

$$\rho' + \rho^e = 0 \quad \dots (4)$$

where  $\rho'$  is the ionic pressure and  $\rho^e$  is the hydrostatic electron-pressure. Putting, the first derivative of ionic-energy in terms of transversal force constant ( $\alpha_1$ ) for nearest neighbours and that ( $\beta_1$ ) for next nearest neighbours, in equation (4), we get

$$\alpha_1 + \beta_1 = -\frac{1}{4} a \rho^e. \quad \dots (5)$$

According to De-Lammy (1956)  $\rho^e = -\frac{3}{5} a K_e$  equation (5) assumes the final form for fcc crystal as

$$\alpha_1 + \beta_1 = -\frac{3}{20} a K_e \quad \dots (6)$$

where  $a$  is the lattice constant and  $K_e$  is the bulk-modulus of the electron-gas.

The elements of dynamical matrix  $|D'_{\alpha\beta}|$  for ion-ion interactions can be written as

$$D'_{\alpha\beta} = -\sum_j \sum_{\mu\nu} \left[ \frac{\partial^2 \phi^i}{\partial x_\alpha \partial x_\beta} \right] \exp(i\mathbf{q} \cdot \mathbf{R}) \quad \dots (7)$$

where

$$\frac{\partial^2 \phi^i}{\partial x_\alpha \partial x_\beta} = \frac{x_\alpha x_\beta}{R_j^3} \left[ \frac{\partial^2 \phi^i}{\partial R_j^2} - \frac{1}{R_j} \frac{\partial \phi^i}{\partial R_j} \right] + \frac{\delta \alpha \beta}{R_j} \frac{\partial \phi^i}{\partial R_j} \quad \dots (8)$$

where  $\alpha, \beta = 1, 2, 3$ . The radial force constants for nearest and next-nearest neighbouring ions are termed as  $\alpha_2$  and  $\beta_2$  respectively and are defined as—

$$\alpha_2 = \left[ \frac{\partial^2 \phi^i}{\partial R_j^2} \right]_{\text{for nearest}} \quad \beta_2 = \left[ \frac{\partial^2 \phi^i}{\partial R_j^2} \right]_{\text{for next nearest}} \quad \dots (9)$$

The transversal force constants for nearest and next nearest ions are termed as  $\alpha_1$  and  $\beta_1$  respectively and are expressed as—

$$\alpha_1 = \left[ \frac{1}{R_j} \frac{\partial \phi^i}{\partial R_j} \right]_{\text{for nearest}} \quad \beta_1 = \left[ \frac{1}{R_j} \frac{\partial \phi^i}{\partial R_j} \right]_{\text{for next nearest}} \quad \dots \quad (10)$$

The elements of dynamical matrix ( $D_{\alpha\beta}^e$ ) due to ion-electron-ion interactions are expressed according to Sharma-Joshi (1963) scheme as

$$D_{\alpha\beta}^e = V q_\alpha q_\beta K_e G^2(qr_0) \quad \dots \quad (11)$$

where  $q_\alpha$ ,  $q_\beta$  are the components of phonon wave vector and

$$G(qr_0) = \frac{3[\text{Sin}(qr_0) - qr_0 \text{Cos}(qr_0)]}{(qr_0)^3} \quad \dots \quad (12)$$

where  $r_0$  is the radius of Wigner-Seitz sphere and is given by the expression

$$\frac{4}{3} \pi r_0^3 = \frac{a^3}{4} \quad \dots \quad (13)$$

The phonon-angular-frequencies ( $\omega$ ) can be computed using the following relation—

$$[D_{\alpha\beta} - m\omega^2 I] = 0 \quad \dots \quad (14)$$

where  $|D_{\alpha\beta}|$  is the total element i.e., sum of ion-ion and ion-electron-ion elements of the dynamical matrix.  $m$  is the mass of the ion and  $I$  is the unit matrix of third order.

### 3. CALCULATIONS

The five force constants ( $\alpha_2$ ,  $\alpha_1$ ,  $\beta_2$ ,  $\beta_1$  and  $aK_e$ ) of the model are computed by using eq. (6) and the following four equations—

$$aC_{11} = 2(\alpha_2 + \alpha_1) + 4\beta_2 + aK_e \quad \dots \quad (15)$$

$$aC_{12} = \alpha_2 - 5\alpha_1 - 4\beta_1 + aK_e \quad \dots \quad (16)$$

$$aC_{44} = \alpha_2 + 3\alpha_1 + 4\beta_1 \quad \dots \quad (17)$$

$$4\pi^2 m v_L^2 = 8(\alpha_2 + \alpha_1) + 0.44 aK_e \quad \dots \quad (18)$$

where  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$  are the elastic stiffness constants of the crystal and  $v_L$  is the known zone-boundary frequency along  $[\xi 00]$  direction.

### 4. INPUT DATA AND RESULTS

The input data and computed force constants for the platinum, lead and thorium are shown in tables 1 and 2 respectively.

Table 1. Input data

Crystal	$C_{11}$	$C_{12}$	$C_{44}$	Ref. for Elastic constants	$a$ in Å	$\nu_L$ in THz	Ref. for zone boundary frequen- cies
Platinum	3.467	2.507	0.767	<i>a</i>	3.9237	4.55	<i>d</i>
Lead	0.495	0.423	0.149	<i>b</i>	4.95	2.07	<i>e</i>
Thorium	0.753	0.489	0.478	<i>c</i>	5.08	3.474	<i>f</i>
<hr/>							
<i>a</i> ) MacFarlane <i>et al</i> (1966)		<i>b</i> ) Kittel (1971)		<i>c</i> ) Allard (1969)			
<i>d</i> ) Ohrlich & Drexel (1968)		<i>e</i> ) Stedman <i>et al</i> (1967)		<i>f</i> ) Reese <i>et al</i> (1973)			

Table 2. Computed force parameters

Crystal	$ak_r$	$\alpha_2$	$\alpha_1$	$\beta_3$	$\beta_1$
in $10^4$ dyn/cm					
Platinum	3.10273	4.7772	-0.1053	0.2916	-0.3601
Lead	0.61650	0.900315	-0.207115	0.11183	0.11461
Thorium	0.02541	2.3639	-0.07961	-0.1922	0.0758

The computed dispersion curves along the high symmetry directions for platinum, lead and thorium are shown in figs. 1, 2 and 3 respectively. The experimental points for platinum, lead and thorium are recently reported by Ohrlich & Drexel (1968), Stedman *et al* (1967) and Reese *et al* (1973) respectively.

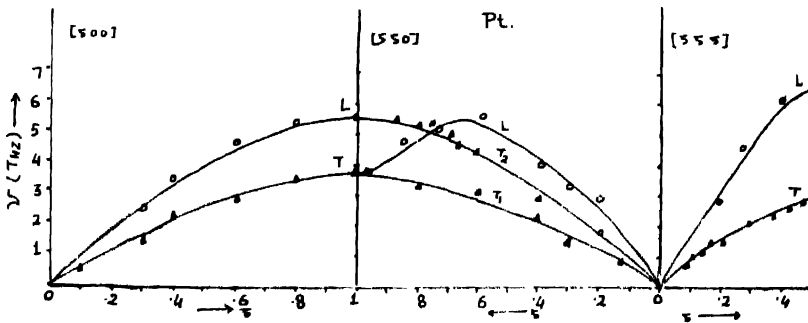


Fig. 1

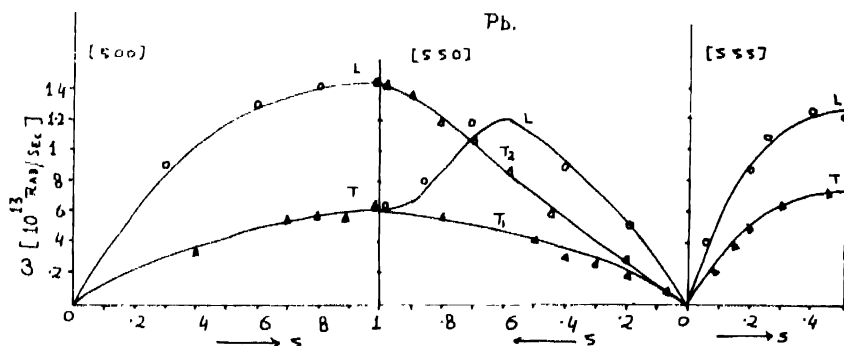


Fig. 2

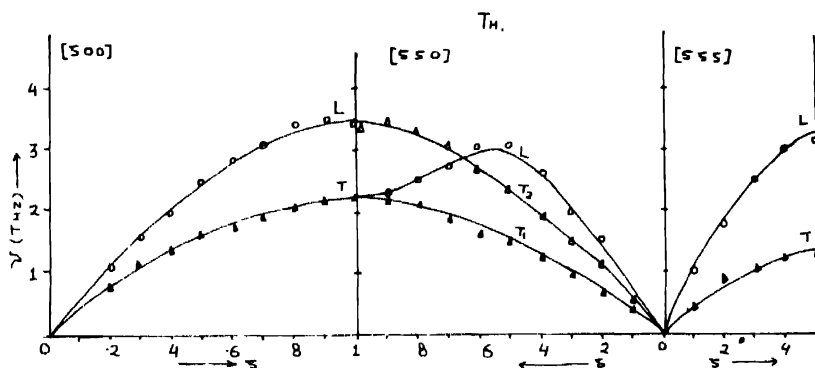


Fig. 3

## 5. DISCUSSION

Most of the phenomenological studies reported till now uses two or more known zone boundary frequencies in their lattice dynamical computations. The present model, being simple requires only one known zone boundary frequency for the successful description of crystal mechanics.

Kont's (1971) study of platinum reveals the large deviation of T-branch along  $[\xi\xi\xi]$  direction. The dispersion frequencies computed so far for mis-behaved crystal lead also shows such deviations from experimental ones. The present model provides a better mathematical frame-work as compared to that reported by Foreman & Lomer (1957). The band structure calculations due to Gupta & Loucks (1969-1971) and those due to Rosengren (1975) show that thorium behaves much like a transition metal. The dispersion frequencies computed on the basis of the present model clearly indicate that the lattice dynamical behaviour of the metals is explained sufficiently well.

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